

Explore Spark for Metagenome assembly

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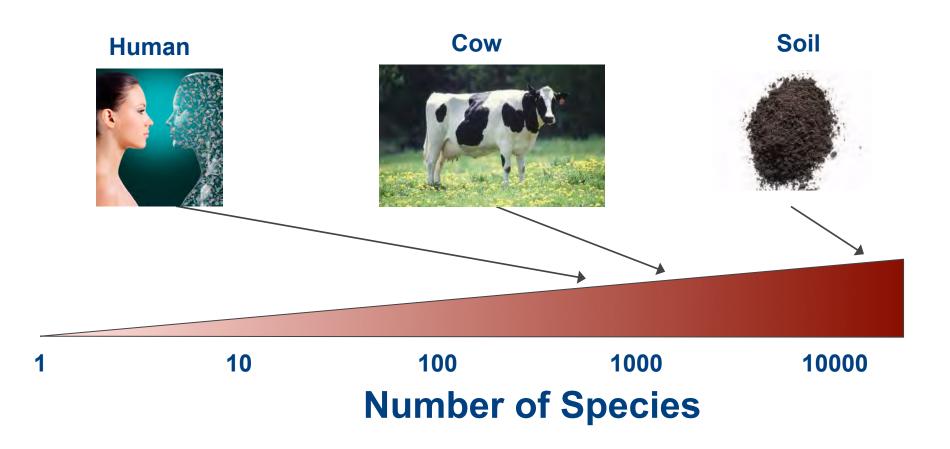
National Microbiome Initiative





Environmental microbial communities are complex



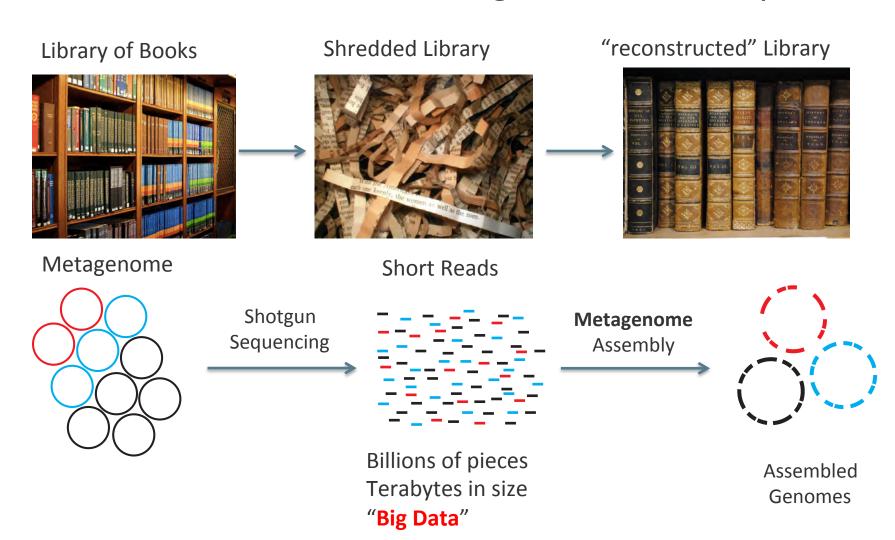


>90% of the species haven't been seen before

Decode Metagenome



Genome ~= Book Metagenome ~= Library



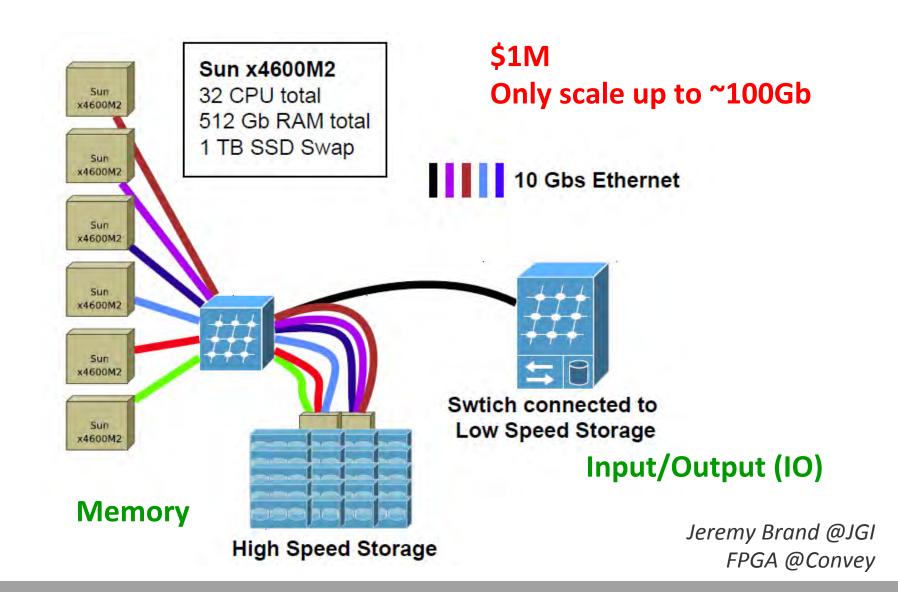
The Ideal Solution



 Easy to develop Robust Scale to big data Efficient

2009: Special Hardware





2010: MP/MPI on supercomputers





MPI version
412 Gb, 4.5B reads
2.7 hours on 128x24 cores
NESRC Supercomputer

Problems:

Fast, scalable

- Experienced software engineers
- Six months of development time
- One task fails, all tasks fail

2011: Hadoop/Map Reduce framework



Google MapReduce

- Data Parallel programming model to process petabyte data
- Generally has a map and a reduce step

Apache Hadoop

- Distributed file system (HDFS) and job handling for scalability and robustness
- Data locality to bring compute to data, avoiding network transfer bottleneck

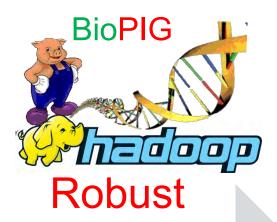
Programmability: Java vs Pig



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2013: BioPig





BioPig-Blaster BioPig-Assembler BioPig-Extender

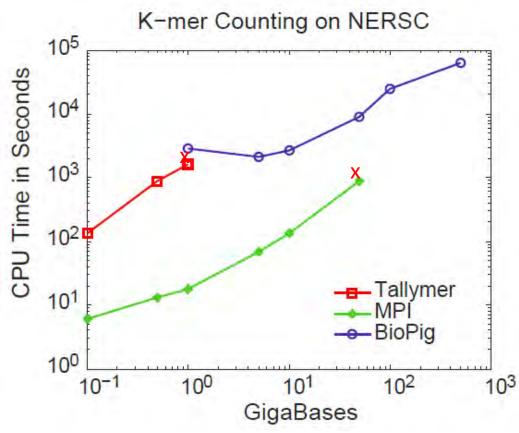
Programmability

BioPig: 61 lines of code

MPI-extender: ~12,000 lines

(vs 31 in BioPig)





Karan Bhatia, Henrik Nordberg, Kai Wang

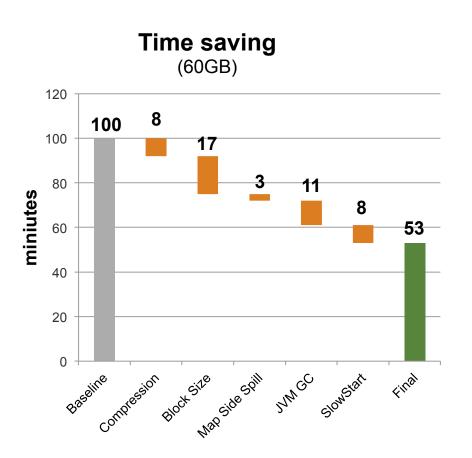
Challenges in application



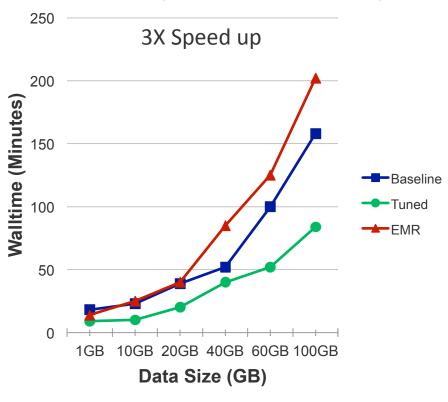
- 2-3 orders of magnitude slower than MPI
- IO optimization, e.g., reduce data copying
- Some problems do not easily fit into map/reduce framework, e.g., graph-based algorithms
- Runs on AWS, but cost \$\$\$ if not optimized

Optimizing BioPig





Still very low efficiency!



Lizhen Shi, Weikuan Yu @FSU

Addressing big data: Apache Spark





- New scalable programming paradigm
 - Compatible with Hadoop-supported storage systems
- Improves efficiency through:
 - In-memory computing primitives
 - General computation graphs
- Improves usability through:
 - Rich APIs in Java, Scala, Python
 - Interactive shell

Goal: Metagenome read clustering



Data characteristics:

- Total data size typically 100Gb 1Tb
- >1 billion short pieces (reads, each 100-200bp)
- >1,000 different species, some species are more similar than others
- Sequence errors 1-2%

Proposed approach: Divide-and-conquer

- Cluster reads from each genome (Clustering)
- Assemble each cluster in parallel (Assembly)

Read clustering with Spark: idea



Local information: overlap

Spark Metagenome

Metagenome Assemb

genome Assembler



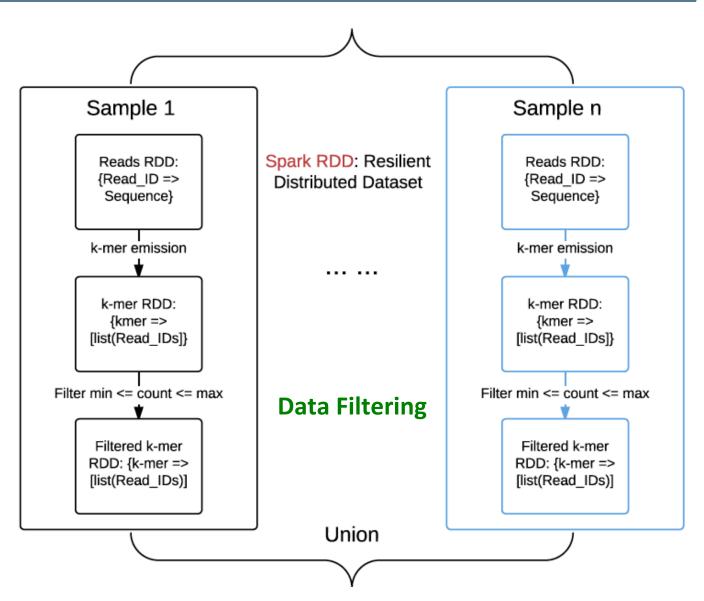
Global information: covariance

Sample1 Sample2 Sample3 10 Spark 1 Spark 2 Spark 10 Metagenome 2 Metagenome 1 Metagenome **10** Assembler 2 Assembler 1 Assembler 5 de 2 de **10** de 5 bruijn 10 bruijn 2 bruijn



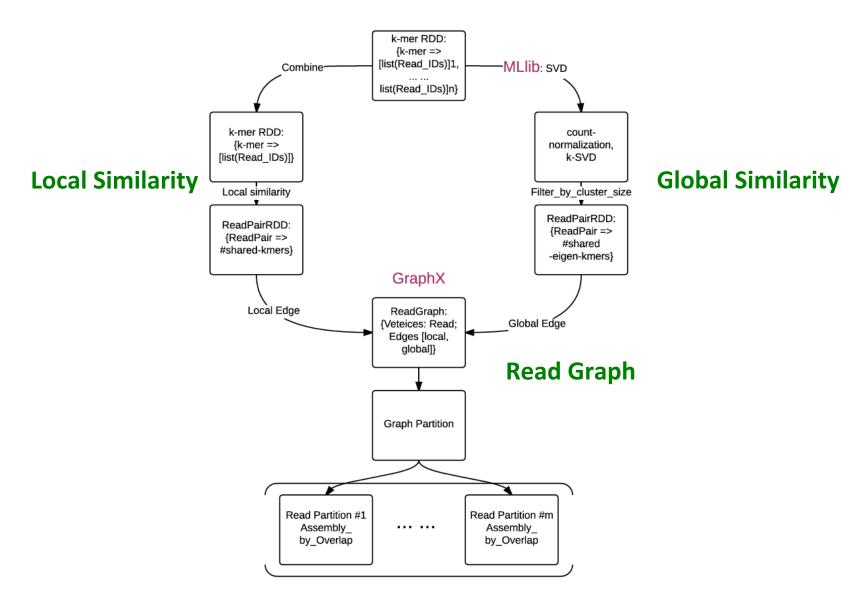
Read clustering with Spark: preprocess





Read clustering with Spark: core





Toy test datasets



- Species:
 - 6 bacterial species
 - Synthetic communities with random proportions of each

Data: single genome sequence data (synthetic & real reads)

Cluster evaluation criteria: NMI



NMI: normalized mutual information

Mutual Information: How pure the different clusters are

$$NMI(\Omega,\mathbb{C}) = \frac{I(\Omega;\mathbb{C})}{[H(\Omega) + H(\mathbb{C})]/2}$$

Entropy: Penalizes having small clusters

Testing Environments

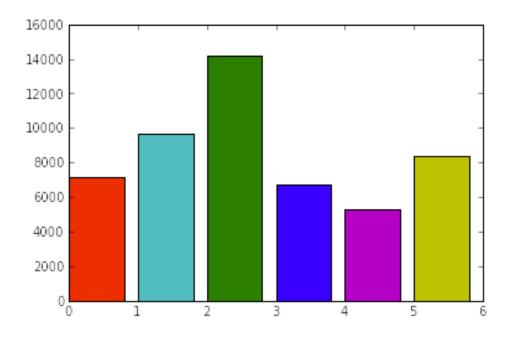


- Local
 - Algorithm development
 - 32-core
 - 256GB memory
- HPC-Lawrencium
 - Small scale analysis
 - CPU: INTEL XEON E5-2670
 - 16-core per node
 - 64GB memory per node
 - Infiniband FDR
- NERSC-Cori
 - Large scale analysis
 - CPU: Cray Haswell
 - 32-core per node
 - 128GB memory per node
 - Cray Aries high-speed interconnect with Dragonfly topology

Local Similarity



In ideal situation (no errors, no repetitive sequences, sufficient sequence coverage): read clustering with local similarity works perfectly.



Reads of the same color belong to the same genome

With real-world situations where:

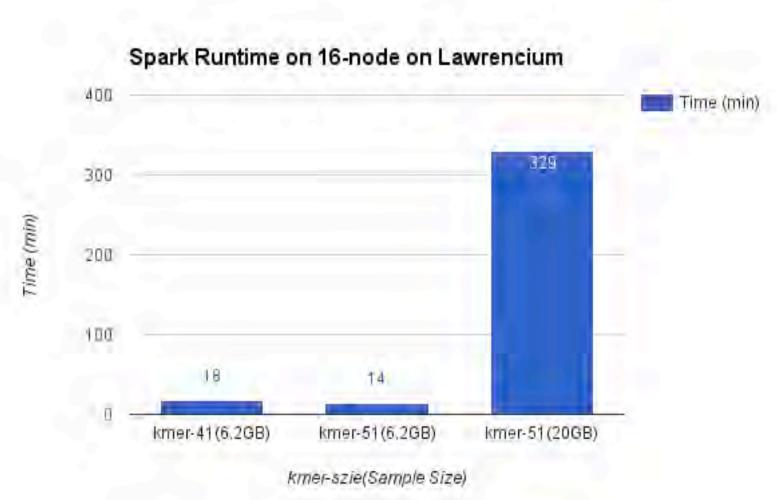
Sequencing coverage is low, many small clusters may form from a same genome, leads to False Negatives

Different genome share sequences, they can fall into the same cluster, leads to

False Positives.

Some performance metrics





Needs 500-700X of memory – optimization is needed

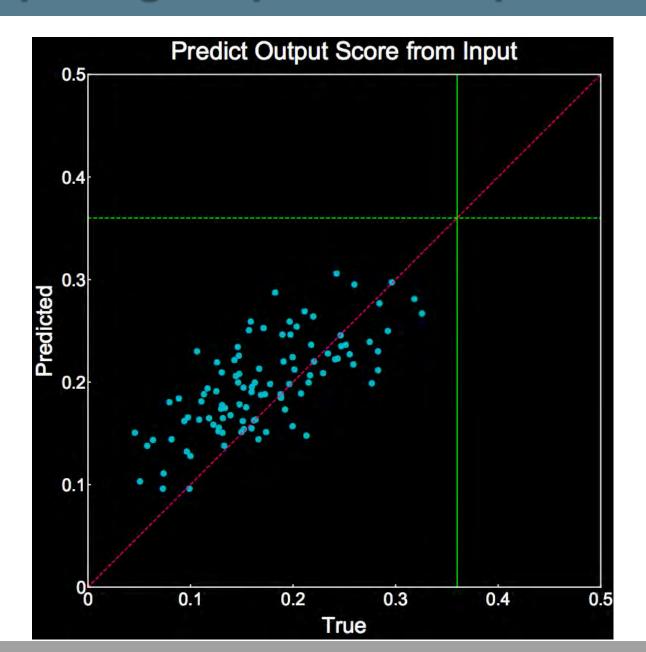
Global Similarity: input Parameters



No samples	1-1000
K-mer Length	20-50
K-Means Clusters	10-500
Eigen K-mers to sample	1-10,000
Eigen Reads to sample	100-60,000
Global Weight	0-150
Power Iteration Clusters	10-150
Power Iteration Steps	0-50

Exploring the parameter space





Jordan Hoffman @Harvard

Overall impression of Spark



- ✓ Easy to develop
- ? Robust
- ? Scale to big data
- ? Efficient
 - VS Hadoop/PIG
 - VS MPI

Acknowledgements



BioPig Team

Henrik Nordberg Kai Wang Karan Bhat @ Amazon Lizhen Shi, Weikuan Yu @ FSU

Spark Team

Xiandong Meng Jordan Hoffman





Lisa Gerhardt , Evan Racah Shane Cannon @ NERSC

Gary Jung, Greg Kurtzer Bernard Li, Yong Qin @ HPC

